



Office of Research and Development  
National Health and Environmental Effects Research Laboratory  
**Mid-Continent Ecology Division (MED)**

**PATRICIA K. SCHMIEDER**

U.S. Environmental Protection Agency  
National Health and Environmental Effects Research Laboratory  
Mid-Continent Ecology Division - Duluth  
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(revised 03/15/02)

**EDUCATION**

<u>Degree</u>	<u>Year</u>	<u>Major</u>	<u>Institution</u>
Ph.D.	1990	Toxicology	Oregon State University, Corvallis, OR
M.S.	1981	Environmental Science	Rutgers University, New Brunswick, NJ
B.S.	1978	Water Science	University of Wisconsin-Stevens Point, WI

**EXPERIENCE**

**Chief, Molecular and Cellular Mechanisms Research Branch/Research Toxicologist**

<u>Dates</u>	<u>Employer</u>
09/00 - Present	U.S. Environmental Protection Agency Mid-Continent Ecology Division Duluth, MN

Brief Description of Position: Branch Chief responsibilities include: obtain and track resources needs and utilization for projects within the Branch; communicate the purpose, progress, and results of within-branch and cross-branch project teams to the Division management, NHEERL management, and EPA Program Offices; network with EPA and professional colleagues to be able to encourage and recognize the application of state-of-the-science approaches to Branch projects; serve on Division-wide, NHEERL-wide, ORD-wide, and Agency-wide planning groups as assigned; bring knowledge of Agency problems back to the Division to guide and inform the direction of research to solve Agency problems; guide and mentor Branch staff to encourage positive working relationships within and outside the Division; advise and guide career development of all Branch personnel; participate as member of Division senior management team to participate in the decision making process to guide the management and research mission of the Division. Continue to promote the scientifically-sound application of QSAR, *in vitro*, and *in vivo* models for the ranking and prioritization and screening of large chemical inventories to address Agency risk assessments needs.

## **Research Toxicologist/Biochemical and Cellular Toxicology Team Leader**

### Dates

06/00 - 09/00

### Employer

U.S. Environmental Protection Agency  
Mid-Continent Ecology Division  
Duluth, MN

Brief Description of Position: Team Leader of Biochemical and Cellular Toxicology Team, Toxic Mechanisms Branch. Team Leader duties include planning, coordinating, facilitating, and conducting research in the areas of species extrapolation to address issues in endocrine disruption research, xenobiotic metabolism, and chemical mode of toxic action. The research approach of the Team focuses on the use of *in vitro* methods at the molecular, biochemical, cellular, and tissue levels of biological organization, and requires directing and coordinating of the activities of eleven scientists including biochemists, toxicologists, cellular biologist, analytical chemists and biologists. Duties include the writing of long-range Research Strategies, writing of detailed Research Plans, coordinating collaborative research efforts with other MED Research Teams, developing interactions with researchers in other NHEERL Divisions, communicating research results to NHEERL science managers, EPA Program Office staff, and the scientific community. Also responsible for allocation of human resources to multiple projects, and identification of, coordination of, and facilitation of team needs for supplies, equipment, space, computing, and library resources. Research: Principal Investigator (PI) on research projects to 1) characterize the toxicodynamics of reactive chemical mode of action for development of mechanistically-based quantitative structure-activity models; 2) characterize metabolic activation reactions in aquatic organisms towards the development of predictive models of xenobiotic metabolism; 3) develop *in vitro* screening methods for assessing the chemical potential for estrogenicity in fish; and 4) demonstrate the utility of small fish models for assessing toxicity of water contaminants including reproduction, development, and cancer. Research interests include: study of electrophile/proelectrophile and receptor binding mechanisms associated with chemical toxicity in aquatic organisms, xenobiotic metabolism, fish toxicokinetics and physiology, and multiple endpoint toxicity assessments.

## **Acting Associate Director for Science**

### Dates

02/00 - 06/00

### Employer

U.S. Environmental Protection Agency  
Mid-Continent Ecology Division  
Duluth, MN

Brief Description of Position: 120-day assignment as Acting Associate Director of Science at MED. Duties include Chair of Research Integration Committee, member of Senior Management Team with Director, Associate Director for Management, and Branch Chiefs. Involved with management policy decisions, direction of scientific planning, participant in budget calculations and allocations. Duties include the technical review and final approval of all scientific planning documents, scientific journal articles, abstracts, and reports. Coordinate, summarize, and report the Division's final technical review of the NHEERL-wide Aquatic Stressors Implementation Plan. Special Projects: Serve on NHEERL Research Support Steering Committee - Develop and report the Division's budgetary needs for NHEERL Research Support (Infrastructure) dollars; Devise implementation strategy for MED Research Plan writing and approval. Determine what plans need to be written and devise tracking method for plan approvals including coordination of Quality of Science Committee, Quality Assurance Committee, Health and Safety Committee, and Animal Care and Use Committee reviews of Research Plans.

## **Research Toxicologist/Biochemical and Cellular Toxicology Team Leader**

### Dates

1995 - 02/00

### Employer

U.S. Environmental Protection Agency  
Mid-Continent Ecology Division  
Duluth, MN

Brief Description of Position: Research Toxicologist and Biochemical and Cellular Toxicology Leader, Toxic Mechanisms Branch. Team Leader duties include coordination of team activities such as development of long-range Strategic Plan, as well as detailed Research Plans, and encourage/pursue collaborative research efforts with other teams and NHEERL Divisions. Also responsible for allocation of human resources to multiple projects, and coordination and facilitation of team needs for supplies, equipment, space, computing, and library resources. Research: PI on research projects to 1) characterize modes of toxic action of reactive chemicals for development of mechanistically-based quantitative structure-activity models; 2) characterize metabolic activation reactions in aquatic organisms; 3) develop *in vitro* screening methods for estrogenicity in fish; and 4) utilization of small fish models for assessing toxicity of water contaminants including reproduction, development and cancer. Research interests include: study of electrophile/proelectrophile and receptor binding mechanisms associated with chemical toxicity in aquatic organisms, xenobiotic metabolism, fish toxicokinetics and physiology, and multiple endpoint toxicity assessments.

## **Research Toxicologist**

### Dates

1990 - 1995

### Employer

U.S. Environmental Protection Agency  
Environmental Research Laboratory  
Duluth, MN

Brief Description of Position: Research Toxicologist, Predictive Toxicology Branch. PI studying toxicodynamics of reactive chemicals in aquatic species. Study includes selection of appropriate biochemical and cellular assays to assess degree of alkylation and redox cycling contributing to cellular toxicity. Requires adaptation of series of mammalian assays for use with aquatic species, development and characterization of *in vitro* models appropriate to research question. Also, Co-PI investigating methods to characterize bioactivation reactions in aquatic species. From 1990-1991 was Co-PI studying chemical dose and bioconcentration in small fish. Primary focus on determination of kinetic rate constants for uptake and elimination of organic chemicals in medaka during short or long-term exposures.

## **Research Aquatic Biologist**

### Dates

1987 - 1989

### Employer

U.S. Environmental Protection Agency  
Environmental Research Laboratory  
Duluth, MN

Brief Description of Position: Research Aquatic Biologist, on IPA with U.S. EPA, ERL-Duluth, and Oregon State University, Hatfield Marine Science Center, Newport, OR. Research on the uptake of organic chemicals across fish gills. Study of the measurement and manipulation of physiological parameters (i.e., fish cardiac output and gill ventilation) to characterize the influence of perfusion and ventilation on organic chemical uptake by fish.

## **Research Aquatic Biologist**

### Dates

1985 - 1987

### Employer

U.S. Environmental Protection Agency  
Environmental Research Laboratory  
Duluth, MN

Brief Description of Position: Research Aquatic Biologist. Conduct fish toxicokinetic and toxicodynamic studies using a variety of organic chemicals. Participate in structure-activity research using fish respiratory-cardiovascular responses to toxic chemicals in a multivariate classification scheme to predict acute toxic mode of action. Participate in research investigating parameters governing chemical uptake and distribution in rainbow trout.

## **Principal Technician**

### Dates

1984 - 1985

### Employer

Department of Pharmacology  
University of Minnesota-Duluth Medical School  
Duluth, MN

Brief Description of Position: Principal Technician. Participate in Cooperative Agreement studies to determine chemical dose accumulated from water exposures, using fish respirometer-metabolism chambers. Participate in planning and execution of studies to monitor physiological responses of rainbow trout to acute doses of a variety of xenobiotics.

## **Junior Scientist**

### Dates

1982 - 1984

### Employer

Center for Lake Superior Environmental Studies  
University of Wisconsin-Superior  
Superior, WI

Brief Description of Position: Junior Scientist. Work on Cooperative Agreement as primary analytical chemist studying uptake, elimination, and tissue distribution of <sup>14</sup>C-labeled organic compounds in rainbow trout using respirometer-metabolism chambers. Member of analytical chemistry team measuring water concentrations of organic compounds for project determining fathead minnow LC50s for a wide variety of organic chemicals.

## **PROFESSIONAL SOCIETIES**

Society of Environmental Toxicology and Chemistry  
International Society for the Study of Xenobiotics  
American Chemical Society  
Society of Toxicology-Northland Chapter

## **AWARDS**

2001 - NHEERL Award, Superior Accomplishment Recognition and Team Award; Initiating collaborative Ecology and Health Division research to evaluate the potential utility of a small fish bioassay to detect adverse outcomes from exposure of trace contaminants in water.

2000 - Superior Accomplishment Recognition and Team Award; Analytical methods development applied to the detection of low levels of glutathione and glutathione conjugates in fish cells.

2000 - Superior Accomplishment Recognition Award; Sustained superior performance in areas of assessing Division infrastructure needs, executing new Divisional research planning process, identifying Division research products, and forging partnerships with other Divisions and EPA Programs.

2000 - Superior Accomplishment Recognition and Team Award; Accomplishments of Acting Senior Managers during extended absence of Division Director.

1999 - Superior Accomplishment Recognition Award; Sustained superior performance.

1999 - Superior Accomplishment Recognition and Team Award; Application of analytical chemistry to identification and quantification of bioactivated metabolites in fish.

1998 - MED Award; Superior accomplishments as MED representative on ORD Human Resources Council.

1997 - ORD Endocrine Disruptor Internal Award Competition; Xenobiotic binding to the estrogen receptor: A comparison of species-specific responses utilizing *in vitro* test systems and quantitative structure-activity relationships.

1993 - EPA Scientific and Technological Achievement Award, Honorable Mention; Blood and water flow limitations on gill uptake of organic chemicals in the rainbow trout (*Onchorynchus mykiss*).

1988 - EPA Scientific and Technological Achievement Award; Use of respiratory-cardiovascular responses of rainbow trout in identifying fish acute toxicity syndromes, Part I and Part II.

1987 - EPA Scientific and Technological Achievement Award; Toxicokinetic modeling of (14)C-PCP in the rainbow trout.

1986 - EPA Scientific and Technological Achievement Award; Absorption dynamics of organic chemical transport across trout gills as related to octanol-water partition coefficient.

## **PROFESSIONAL ACTIVITIES/APPOINTMENTS**

### **Research Experience**

Develop models to predict chemical toxicological potential (2-D and 3-D SAR/QSAR) for ranking and prioritization of large chemical inventories. Risk assessment application of small fish models for prediction of impaired reproduction, development, and cancer upon exposure to water contaminants. Develop *in vitro* assays and 3-D SAR models to screening EDCs. Develop and apply *in vitro* methods to assess metabolism and bioactivation rates in fish. Develop and apply methods to differentiate electrophile/pro-electrophile reactivity in fish. Develop analytical approaches to quantify glutathione species and conjugates at trace levels in fish. Quantify bioconcentration factor of dioxin in medaka. Develop *in vivo* blood flow probe technique for measurement of cardiac output, liver perfusion, etc. for physiologically-based fish models. Develop fish acute toxicity syndrome approach to differentiate chemical modes of action for development of mechanistically-based QSAR models. Characterize pentachlorophenol toxicokinetics and metabolism in fish; measurement and descriptive modeling of organic chemical absorption at fish gills.

### **National and International Activities**

2001 - Invited participant, International Workshop on Standardization of Endocrine-Disrupters Testing in Medaka, June 6-8, 2001, Nagoya, Japan.

2000 - Invited presentation, "A 3-D QSAR-based identification algorithm for potential estrogen receptor ligands," Bradbury, S., P. Schmieder, G. Ankley, O. Mekenyan, and V. Kamenska. 9th International Workshop on Quantitative Structure-Activity Relationships in Environmental Sciences, September 16-20, Bourgas, Bulgaria. (Presented by P. Schmieder.)

2000 - Invited participant, International Symposium on Endocrine-Disrupting Substance Testing in Medaka, March 17-20, Nagoya, Japan.

2000 - Invited participant, 2nd International "Organization for Economic Cooperation and Development (OECD) Expert Consultation on Testing in Fish," March 15-16, Tokyo, Japan.

2000 - Invited participant, "Risk Assessment for Human Health and the Environment," SETAC-Europe, May 21-25, Brighton, UK. (Unable to attend due to unavailability of EPA travel funds.)

1999 - Invited participant, "USEPA Drinking Water Needs Expert Workshop," September 27-29, Leesburg, VA.

1999 - Invited to present paper at Aquatic Mechanism of Action Research Session, SETAC-Europe, May 1999, Leipzig, Germany. (Unable to attend due to unavailability of EPA travel funds.)

1998 - Invited participant, International "Organization for Economic Cooperation and Development (OECD) Expert Consultation on Testing in Fish," October 28-29, London, UK.

1998 - Invited participant, USEPA Harmful Algal Bloom Workshop, October 6-7, 1997, Pensacola Beach, FL.

1997 - Invited plenary presentation, "Endocrine Disruption in Wildlife Species: Research and Policy," 24th Annual Aquatic Toxicity Workshop, October 19-22, 1997, Niagara Falls, Ontario, Canada.

1997 - Invited participant, IEH Workshop on Assessment of the Ecological Significance of Sex Hormone Disruption. Sponsored by Institute for Environment and Health, May 28-30, Leicester, UK.

#### **U.S. EPA Committees**

Member NHEERL Goal 4 "Safe Communities" Implementation Steering Committee - Division representative on committee to identify toxics and pesticides priority research areas, and guide the development of cross-divisional research plans to address the needs of OPPTS (January 2001 - Present)

Member NHEERL Infrastructure Steering Committee - MED representative on advisory group to NHEERL senior management, making budgetary recommendations for allocation of research support (infrastructure) funds across NHEERL Divisions (August 2000 - Spring 2001)

Member NHEERL CCL Workgroup - MED representative on research planning group to address Office of Drinking Water research needs for chemicals on Contaminant Candidate List (CCL-I) (October 1999 - 2000)

ORD-Human Resource Council - MED representative on ORD-wide committee to identify human resource issues and make recommendations to the Assistant Administrator for Office of Research and Development (1996 - 1998)

Co-Chair Chemical Extrapolations Committee - In-lab planning committee to discuss research needed to improve EPA's ability to extrapolate limited chemical toxicity data to predict ecological impact of untested chemicals, for use in ecological risk assessments. Committee output from this research planning effort serves as basis for formation of MED Research Teams, MED, Duluth, MN (1995)

NHEERL Organizational Task Force - Committee participant in two-day workshop, Washington, DC (1994)

Co-Chair Strategic Integration Committee - In-lab planning committee to address coordination of research efforts within ERL-D to maximize efficiency of resources, reduce redundancy in efforts, and strengthen and enhance research accomplishments through integrated research efforts, ERL, Duluth, MN (1994)

Chair ERL-D Seminar Committee, ERL, Duluth, MN (1992)

Member Animal Care and Welfare Committee - Ad-hoc committee responsible for writing ERL-D Animal Care and Use Plan, ERL, Duluth, MN (1992)

### **National and International Cooperative Research Projects**

Collaboration on "Structure-Activity Evaluation of Gene Activation" with Prof. J. Sumpter, Dept. of Biology and Biochemistry, Brunel University, Uxbridge, Middlesex, UK; and Prof. O. Mekenyan, Dept. Physical Chemistry, Univ. "Prof. A. Zlatarov," Bourgas, Bulgaria (1998 - 2000)

Current collaboration on "Xenobiotic Binding to the Estrogen Receptor: A Comparison of Species-Specific Responses Utilizing *In Vitro* Test Systems and Quantitative Structure-Activity Relationships," with L.E. Gray, EPA, ORD, NHEERL, Reproductive Toxicology Division, Research Triangle Park, NC (1997 - Present)

Hosted pre-doctoral candidate, Enaut Urrestarazu Ramos, Research Institute of Toxicology, Utrecht University, Utrecht, The Netherlands. He cooperated with our group on investigating the application of microdialysis and membrane disc absorption binding techniques to the quantitation of available chemical fraction in studies with reactive quinones (1996)

### **Project Officer U.S. EPA Grants and Cooperative Agreements**

2001 - 2003 Mekenyan, O., "Methods for Identifying Chemicals That Elicit Adverse Biological Effects," CR828823-01.

1997 - 1999 Mekenyan, O., "Stereochemical Factors: Issues in Chemical Reactivity and Ecotoxicology," CR822306-1, University "Prof. A. Zlatarov," Bourgas, Bulgaria.

1995 - 1997 Cech, J., "Bioavailability of Mercury in the Presence of Humic Substances in Clear Lake," CR-824192-01, University of California-Davis, Davis, CA.

### **Teaching and Mentoring**

Co-Research Advisor for NRC Post-doctoral Fellow, Dr. M. Hornung, "Development of a Fish Cell Assay System to Screen Environmental Chemicals for Estrogen Receptor Activation" (1998 - 2001)

Co-Research Advisor for NRC Post-doctoral Fellow, Dr. L. Solem, "Validation of fish PB-TK Modeling for Xenobiotics which Undergo Metabolic Transformation" (1997 - 2000)

Research Advisor to Undergraduate Student Intern, K. Keough, in the University of Minnesota-Duluth Ni-Shou-Gabawag Minorities into Biomedical Research Support Program (1992 - 1994)

Invited participant in an Aquatic Toxicology Workshop, Oregon State University, Hatfield Marine Science Center, Newport, Oregon, June 20-25 (1988)

Invited participant in an Aquatic Toxicology Workshop, Oregon State University, Hatfield Marine Science Center, Newport, Oregon, June 13-17 (1987)

### **Workshops**

2002 - Chaired Organizing Committee, Risk Assessment Forum Sponsored Workshop on Use of Small Fish (Medaka) Data in Risk Assessment, June 11-13, Duluth, MN.

2001 - Chaired Session on Discussion of Test Designs, International Workshop on Standardization of Endocrine-Disrupters Testing in Medaka, June 6-8, Nagoya, Japan.

2000 - Chaired Organizing Committee, First International James M. McKim Species Extrapolation Workshop, October 28, Duluth, MN.

## PUBLICATIONS

### Peer-Reviewed Journals

Mekenyan, O., N. Nikolova, and P. Schmieder. 2002. Dynamic 3D QSAR techniques: Applications in toxicology. Theoretical Chemistry (in press).

Schmieder, P., G. Ankley, O. Mekenyan, J. Walker, and S. Bradbury. 2002. QSAR models for predicting ER binding affinity of structurally diverse chemicals. Environ. Toxicol. Chem. (submitted).

Schmieder, P.K., Y. Koleva, and O.G. Mekenyan. 2002. A reactivity pattern for discrimination of ER agonism and antagonism based on 3-D molecular attributes. SAR/QSAR Environ. Res. (in press).

Ankley, G.T., O.G. Mekenyan, V.B. Kamenska, P.K. Schmieder, and S.P. Bradbury. 2002. Reactivity profiles of ligands of mammalian retinoic acid receptors: A preliminary COREPA analysis. SAR/QSAR Environ. Res. (in press).

Hornung M.W., P.K. Schmieder, and G.T. Ankley. 2001. Demonstration of cross-well contamination by estrogen in an estrogen-responsive reporter gene assay. In Vitro Cell Mol. Biol. (submitted).

Schmieder, P.K., A.O. Aptula, E. J. Routledge, J.P. Sumpter, and O.G. Mekenyan. 2000. Estrogenicity of alkylphenolic compounds: A 3-D structure activity evaluation of gene activation. Environ. Toxicol. Chem. 19(7):1727-1740.

Bradbury, S., V. Kamenska, P. Schmieder, G. Ankley, and O. Mekenyan. 2000. A computationally-based identification algorithm for estrogen receptor ligands. Part I. Predicting hER $\alpha$  binding affinity. Toxicol. Sci. 58:253-269.

Mekenyan, O., V. Kamenska, P. Schmieder, G. Ankley, and S. Bradbury. 2000. A computationally-based identification algorithm for estrogen receptor ligands. Part II. Evaluation of a hER $\alpha$  binding affinity model. Toxicol. Sci. 58:270-281.

Tapper, M.A., B.R. Sheedy, D.E. Hammermeister, and P.K. Schmieder. 2000. Depletion of cellular protein thiols as an indicator of arylation in isolated trout hepatocytes exposed to 1,4-benzoquinone. Toxicol. Sci. 55:327-334.

Schmieder, P., M. Tapper, A. Linnun, J. Denny, R. Kolanczyk, and R. Johnson. 2000. Optimization of a precision-cut trout liver tissue slice assay as a screen for vitellogenin induction: Comparison of slice incubation techniques. Aquat. Toxicol. 49:251-268.

Hammermeister, D.E., J. Serrano, P. Schmieder, and D. Kuehl. 2000. Characterization of dansylated glutathione, glutathione disulfide, cysteine, and cystine by narrow bore liquid chromatography - electrospray ionization mass spectrometry. Rapid Commun. Mass Spec. 14(6):503-508.

Kolanczyk, R., P. Schmieder, S. Bradbury, and T. Spizzo. 1999. Pathway and rate of 4-methoxyphenol metabolism in microsomes of rainbow trout (*Oncorhynchus mykiss*). Aquat. Toxicol. 45:47-61.

Schmieder, P., D. Lothenbach, J. Tietge, R. Erickson, and R. Johnson. 1995. [3H]2,3,7,8-TCDD uptake and elimination kinetics in medaka (*Oryzias latipes*). Environ. Toxicol. Chem. 14(10):1735-1743.

Schmieder, P.K. and L.J. Weber. 1992. Blood and water flow limitations on gill uptake of organic chemicals in the rainbow trout (*Oncorhynchus mykiss*). Aquat. Toxicol. 24:103-122.



Schmieder, P.K. and Henry, T.R. 1988. Plasma binding of n-butanol, phenol, nitrobenzene, and pentachlorophenol in rainbow trout and rat: A comparative study. *Comp. Biochem. Physiol.* 91C(2):413-418.

McKim, J.M., P.K. Schmieder, G.J. Niemi, R.W. Carlson, and T.R. Henry. 1987. Use of respiratory-cardiovascular responses of rainbow trout (*Salmo gairdneri*) in identifying fish acute toxicity syndromes. Part II. Malathion, carbaryl, acrolein, and benzaldehyde. *Environ. Toxicol. Chem.* 6:313-328.

McKim, J.M., P.K. Schmieder, R.W. Carlson, E.P. Hunt, and G.J. Niemi. 1987. Use of respiratory-cardiovascular responses of rainbow trout (*Salmo gairdneri*) in identifying fish acute toxicity syndromes. Part I. Pentachlorophenol, 2,4-dinitrophenol, tricaine methanesulfonate, and 1-octanol. *Environ. Toxicol. Chem.* 6:295-312.

McKim, J.M., P.K. Schmieder, and R.J. Erickson. 1986. Toxicokinetic modeling of 14C-pentachlorophenol in the rainbow trout (*Salmo gairdneri*). *Aquat. Toxicol.* 9:59-80.

McKim, J.M., P.K. Schmieder, and G. Veith. 1985. Absorption dynamics of organic chemical transport across trout gills as related to octanol-water partition coefficient. *Toxicol. Appl. Pharmacol.* 77:1-10.

### **Peer-Reviewed Book Chapters/Symposium Proceedings**

Schmieder, P.K. and R. Johnson. 2000. Overview of ecotoxicology research programs and medaka research at the U.S. EPA National Health and Environmental Effects Laboratory's Mid-Continent Ecology Division. In: *Proceedings of an International Symposium: Endocrine-disrupting Substance Testing in Medaka*, March 17-20, Nagoya, Japan. p.113-114.

Tietge, J., R. Johnson, P. Schmieder, and K. Jensen. 2000. Comparative sensitivity of different life-stages of medaka and salmonid fishes to 2,3,7,8-TCDD. In: *Proceedings of an International Symposium: Endocrine-disrupting Substance Testing in Medaka*, March 17-20, Nagoya, Japan. p.53-54.

McKim, J.M. and P.K. Schmieder. 1991. Bioaccumulation: Does it reflect toxicity? In: Nagel, R. and Laskill, R. (eds.), *VCH Verlagsgesellschaft, Weinheim, New York*. p.167-181.

### **INVITED PRESENTATIONS**

Mekenyan, O., P.K. Schmieder, and S.P. Bradbury. 2002. New 3-D techniques for ranking and prioritization of chemical inventories. Workshop - Effectiveness of QSAR for Prescreening of Endocrine Disruptor Hazard. SCOPE/IUPAC International Symposium on Endocrine Active Substances, November 17-21, Yokohama, Japan.

Schmieder, P.K., S.P. Bradbury, G.T. Ankley, and O.G. Mekenyan. 2000. The use of structure-activity relationships in integrating the chemistry and toxicology of endocrine disrupting chemicals. 21st Annual SETAC Meeting, November 12-16, Nashville, TN.

Schmieder, P.K. 2000. Overview of ecotoxicology research at EPA's Mid-Continent Ecology Division Research Laboratory. Annual Meeting of Federal/State Toxicology Risk Analysis Committee, May 22-24, Minneapolis, MN.

Schmieder, P.K., K. Jensen, R. Johnson, and J. Tietge. 2000. Comparative sensitivity of different life-stages of medaka and salmonid fishes to 2,3,7,8-TCDD. International Symposium on Endocrine-Disrupting Substance Testing in Medaka, March 17-20, Nagoya, Japan.

Schmieder, P.K. 2000. Overview of ecotoxicology research at the U.S. EPA NHEERL Mid-Continent Ecology Division. International Symposium on Endocrine-Disrupting Substance Testing in Medaka, March 17-20, Nagoya, Japan.

Schmieder, P.K. 1999. Toxicology and ecology at EPA's Mid-Continent Ecology Division. Northland Chapter of Society of Toxicology, October 20, 1999, St. Paul, MN.

Bradbury, S.P., G.T. Ankley, P.K. Schmieder, and O.G. Mekenyan. 1999. New developments in hazard identification algorithms for hormone receptor ligands. 20th Annual SETAC Meeting, November 14-18, Philadelphia, PA. (Presented by P. Schmieder.)

Schmieder, P.K. 1998. U.S. EPA/ORD research supporting development of a fathead minnow screening assay for endocrine disrupters. OECD Expert Consultation on Testing in Fish, October 28-29, London, UK.

Schmieder, P.K. 1997. Endocrine disruption in wildlife species: Research and policy. Plenary presentation, 24th Annual Aquatic Toxicity Workshop, October 19-22, 1997, Niagara Falls, Ontario, Canada.

Schmieder, P.K., D. Hammermeister, R. Kolanczyk, A. Hoffman, G. Lien, M. Tapper, and R. Johnson. 1996. Differentiating biochemical mechanisms of toxicity for substituted 1,4-naphthoquinones using rainbow trout hepatocytes. Mechanisms and Modes of Action Session, 17th Annual SETAC Meeting, November 1996, Washington, DC.

McKim, J.M. and P.K. Schmieder. 1990. Bioaccumulation. Does it reflect toxicity? International Workshop on Contributions to the Assessment of Bioaccumulation of Organic Chemicals in Aquatic Systems, Berlin, Germany.

McKim, J.M. and P.K. Schmieder. 1986. Dose-response models: Use of fish for study of water-borne toxic agents. Invited paper, American Association for the Advancement of Science Symposium on the Use of Non-mammalian Animal Models in Research and Testing.

#### **FIRST AUTHOR PRESENTATIONS**

Schmieder, P.K., Y.K. Koleva, and O.G. Mekenyan. 2000. A reactivity pattern for discrimination of ER agonism and antagonism based on 3-D molecular attributes. QSAR2000, September 16-21, Bourgas, Bulgaria.

Schmieder, P.K., S.P. Bradbury, C.R. Russom, and S.P. Broderius. 2000. Aquatic toxicity mode of action studies applied to QSAR development. Annual Meeting American Chemical Society, August 20-24, Washington, DC.

Schmieder, P.K., T.R. Henry, and M.W. Hornung. 1999. An *in vitro* screening approach for environmental estrogens: From receptor to tissue. 20th Annual SETAC Meeting, November 14-18, Philadelphia, PA.

Tapper, M., A. Linnum, M. Pasha, J. Korte, J. Denny, R. Johnson, and P.K. Schmieder, P. 1999. A rainbow trout tissue slice assay for screening environmental estrogens. 20th Annual SETAC Meeting, November 14-18, Philadelphia, PA. (Presented by P. Schmieder.)

Hornung, M.W., P.K. Schmieder, and G.T. Ankley. 1999. Development of an environmental estrogen screen using transiently transfected rainbow trout cell lines. 20th Annual SETAC Meeting, November 14-18, Philadelphia, PA.

Schmieder, P.K., M.A. Tapper, A. Linnum, and R.D. Johnson. 1999. Vitellogenin induction in trout liver slices exposed to 17- $\beta$ -estradiol: A comparison of two incubation conditions. *The Toxicologist* 48(1-S):1782.

Schmieder, P., O. Mekenyan, A. Aptula, E. Routledge, and J. Sumpter. 1998. Estrogenicity of alkylphenolic compounds: SAR evaluation of gene activation. Abstract/Oral presentation, 8th International Workshop on Quantitative Structure-Activity Relationships in the Environmental Sciences, May 16-20, Baltimore, MD.

Schmieder, P., R. Kolanczyk, and S.P. Bradbury. 1998. O-dealkylation of 4-methoxyphenol by rainbow trout microsomes. 4th NHEERL Symposium on Extrapolation in Human Health and Ecological Risk Assessments, April 27-30, Cary, NC.

Schmieder, P., R. Kolanczyk, P. Fitzsimmons, K. Keogh, T. Spizzo, D. Hammermeister, A. Hoffman, and R. Johnson. 1994. Differential toxicity of menadione and menadione sodium bisulfite in rainbow trout hepatocytes. 33rd Annual Meeting of the Society of Toxicology, Dallas, TX.

Schmieder, P.K., D. Lothenbach, R. Johnson, R. Erickson, and J. Tietge. 1992. Uptake and elimination kinetics of 3H-TCDD in medaka. 31st Annual Meeting of the Society of Toxicology, Seattle, WA.

Schmieder, P.K. and L.J. Weber. 1991. Blood and water flow limitations on gill uptake of butanol and decanol in the rainbow trout. 30th Annual Meeting of the Society of Toxicology, Dallas, TX.

Schmieder, P.K., R.D. Johnson, and S.P. Bradbury. 1990. Validation of the medaka carcinogenesis model: Phase 2 - Establishing delivered dose. Carcinogenicity Research Review, Department of the Army, Research Methods Branch, Frederick, MD.

Schmieder, P.K. and L.J. Weber. 1989. Influence of trout gill respiratory physiology on kinetics of chemical flux. 10th Annual SETAC Meeting, Toronto, Canada.

Schmieder, P.K. and J.M. McKim. 1984. Understanding dose concepts in fish toxicology. 5th Annual SETAC Meeting Abstracts, p.11.

## **OTHER**

### **Co-authored Abstracts**

Kolanczyk, R.C., P.N. Fitzsimmons, J.M. McKim, and P.K. Schmieder. 2001. Effects of anesthesia (MS222) on liver biotransformation in rainbow trout (*Oncorhynchus mykiss*). The Toxicologist 60(1):462.

Sheedy, B.R., M.A. Tapper, M.W. Hornung, R.C. Kolanczyk, and P.K. Schmieder. 2001. Methoxychlor metabolism and vitellogenesis in male rainbow trout liver slices. The Toxicologist 60(1):173.

Henry, T.R., J.S. Denny, and P.K. Schmieder. 2001. Relative binding affinity of alkylphenols to rainbow trout estrogen receptor. The Toxicologist 60(1):781.

Bradbury, S.P., P.K. Schmieder, G.T. Ankley, O.G. Mekenyan, and V. Kamenska. 2000. A 3-D QSAR-based identification algorithm for potential estrogen receptor ligands. Oral presentation, QSAR2000, September 16-21, Bourgas, Bulgaria. (Presented by P.K. Schmieder.)

Ankley, G.T., V. Kamenska, S. Bradbury, P. K. Schmieder, and O. Mekenyan. 2000. Reactivity profile of conformationally-flexible retinoid receptor ligands. Abstract/Poster presentation, QSAR2000, September 16-21, Bourgas, Bulgaria. (Presented by P.K. Schmieder.)

Henry, T.R., M.W. Hornung, J.S. Denny, M. Tapper, B.R. Sheedy, and P.K. Schmieder. 2000. An *in vitro* approach for screening environmental endocrine disruptors in rainbow trout. Abstract presentation, Gordon Research Conference on Environmental Endocrine Disruptors, June 18-23, Plymouth, NH.

Henry, T., J. Denny, and P. Schmieder. 2000. Non-mammalian estrogenicity screen: Rainbow trout estrogen receptor binding. The Toxicologist 54(1):1530.

Kolanczyk, R., L. Solem, A. Hoffman, P. Schmieder, and J. McKim. 2000. Sex-linked changes in phase I biotransformation of phenol in brook trout over an annual reproductive cycle. The Toxicologist 54(1):1766.

Solem, L., R. Kolanczyk, P. Schmieder, and J. McKim. 2000. Gender specific alteration of glucuronidation in brook trout during the annual reproductive cycle. The Toxicologist 54(1):1765.

Bradbury, S.P., G.T. Ankley, P.K. Schmieder, and O.G. Mekenyan. 1999. New developments in hazard identification algorithms for hormone receptor ligands. Abstract/Oral presentation, 20th Annual SETAC Meeting, November 14-18, Philadelphia, PA. (Presented by P. Schmieder.)

Hornung, M.W., P.K. Schmieder and G.T. Ankley. 1999. Development of an environmental estrogen screen using transiently transfected rainbow trout cell lines. 20th Annual SETAC Meeting, November 14-18, Philadelphia, PA.

Tapper, M., A. Linnum, M. Pasha, J. Korte, J. Denny, R. Johnson, and P. Schmieder. 1999. A rainbow trout tissue slice assay for screening environmental estrogens. 20th Annual SETAC Meeting, November 14-18, Philadelphia, PA.

Pasha, M.S., J. Korte, M. Kahl, K. Jensen, M. Tapper, M. Hornung, P. Schmieder, and G. Ankley. 1999. Development of screening methods for endocrine-disrupting chemicals (EDCs). Annual Meeting of American Chemical Society, August, New Orleans, LA.

Henry, T.R., R.D. Johnson, D.B. Lothenbach, and P.K. Schmieder. 1999. Autofluorescence in primary rainbow trout hepatocytes interferes with measurement of oxidative activity via the exogenous probe, DCF, but provides intrinsic measure of cellular oxidative state. *The Toxicologist* 48(1-S):963.

Hornung, M.W., Korte, J.J., Tapper, M.A., Lambright, C.R., Kelce, W.R., Schmieder, P.K., Gray, L.E., Jr., and G.T. Ankley. 1999. Use of a rainbow trout hepatoma cell line (RTH-149) for screening estrogenic chemicals: Comparison of transfection methods and optimization of reporter activation. *The Toxicologist* 48(1-S):1781.

Hornung, M.W., Tapper, M.A., Korte, J.J., Denny, J.S., Pasha, M.S., Henry, T.R., Schmieder, P.K., and Ankley, G.T. 1999. Development of a multi-level environmental estrogen screen in rainbow trout. Annual Meeting of the Midwest Regional Chapter of the Society of Environmental Toxicology and Chemistry, La Crosse, WI.

Kolanczyk, R.C., L.E. Solem, P.K. Schmieder, and J.M. McKim. 1999. Characterization of hydroquinone and catechol formation using hepatic microsomes from three species of fish. *The Toxicologist* 48(1-S):1234.

Sheedy, B.R. and P.K. Schmieder. 1999. Differences in hepatic vitamin E concentrations in three fish species. *The Toxicologist* 48(1-S):1237.

Solem, L.E., R.C. Kolanczyk, P.K. Schmieder, and J.M. McKim. 1999. *In vivo* microdialysis in a comparative study of hepatic metabolism of phenol in three fish species. *The Toxicologist* 48(1-S):1075.

Tapper, M.A., A. Linnum, M. Pasha, J. Korte, J. Denny, and P.K. Schmieder. 1999. Induction and inhibition of vitellogenin protein synthesis in rainbow trout liver slices upon exposure to estrogens and anti-estrogens. *The Toxicologist* 48(1-S):1783.

Hammermeister, D.E., J. Serrano, P.K. Schmieder, and D.W. Kuehl. 1998. LC/ESI/MS and MS/MS characterization of the dansylated thiols of cysteine, cystine, and reduced and oxidized glutathione. *The Toxicologist* 42(1-S):1073.

Kolanczyk, R.K., P. K. Schmieder, and S.P. Bradbury. 1998. O-dealkylation of 4-methoxyphenol by rainbow trout hepatic microsomes. *The Toxicologist* 42(1-S):1620.

Serrano, J., D.E. Hammermeister, P.K. Schmieder, and D.W. Kuehl. 1998. LC/ESI/MS and MS/MS techniques for the characterization of GSH conjugates of reactive quinones. *The Toxicologist* 42(1-S):1073.

Tapper, M.A., P.K. Schmieder, R.C. Kolanczyk, D.E. Hammermeister, and R.D. Johnson. 1996. Depletion of protein thiols by naphthoquinone in isolated rainbow trout hepatocytes. 17th Annual SETAC Meeting Abstracts, p. 132.

McKim, J.M. and P.K. Schmieder. 1986. Dose-response models: Use of fish for the study of water-borne toxic agents. In: *The Use of Nonmammalian Animal Models in Research and Testing Symposia* (8-3). Abstracts of papers presented, 152nd National Meeting of the American Association for the Advancement of Science, p. 45.

McKim, J. M., P.K. Schmieder, R. Carlson, and E. Hunt. 1984. The use of fish respiratory-cardiovascular responses as an aid in predicting the acute toxic mode of action for selected chemicals. 5th Annual SETAC Meeting Abstracts, p. 45.

McKim, J. M., P.K. Schmieder, and G.D. Veith. 1983. Total flux of selected organic chemicals across trout gills as related to octanol/water partition coefficient. 4th Annual SETAC Meeting Abstracts, p.141.

### **Planning Meetings and Workshops**

NHEERL Research Planning Meeting on Computational Toxicology Initiative, February 2002, Research Triangle Park (RTP), NC.

NHEERL Briefing of OW and OW/OST on progress of medaka water contaminant research. August 2001, RTP, NC.

NHEERL Synergy Workshop on “Medaka as Model for Assessment of Effects of Water Contaminants,” August 2001, RTP, NC.

NHEERL Synergy Workshop on “Extrapolation of Toxicological Effects Among Species: Collaborative Research in the NHEERL EDC Program,” August 8-9, 2000, Duluth, MN.

EPA’s Contaminant Candidate List Research Needs Expert Workshop, September 27-29, 1999, Washington, DC.

NHEERL Extrapolations Workshop, “Toxicological Extrapolation Across Species: Collaborative Opportunities and Needs Within NHEERL Human Health and Ecology Divisions,” August 10-12, 1999, RTP, NC. Participated in HAB and Cancer Models Breakout Groups.

NHEERL Synergy Workshop on “Alternative Models for Assessing Cancer and Developmental Risk of Exposure to By-products of Drinking Water Disinfection-II,” June, 1999, Duluth, MN.

NHEERL Synergy Workshop on “Alternative Models for Assessing Cancer and Developmental Risk of Exposure to By-products of Drinking Water Disinfection-I,” November 1998, Duluth, MN.

4th International Conference on Toxic Cyanobacteria, September 27-October 1, 1998. Participant. CCL Research Needs Expert Workshop, September 27-29, 1999, Washington, DC.